

FIG. 4

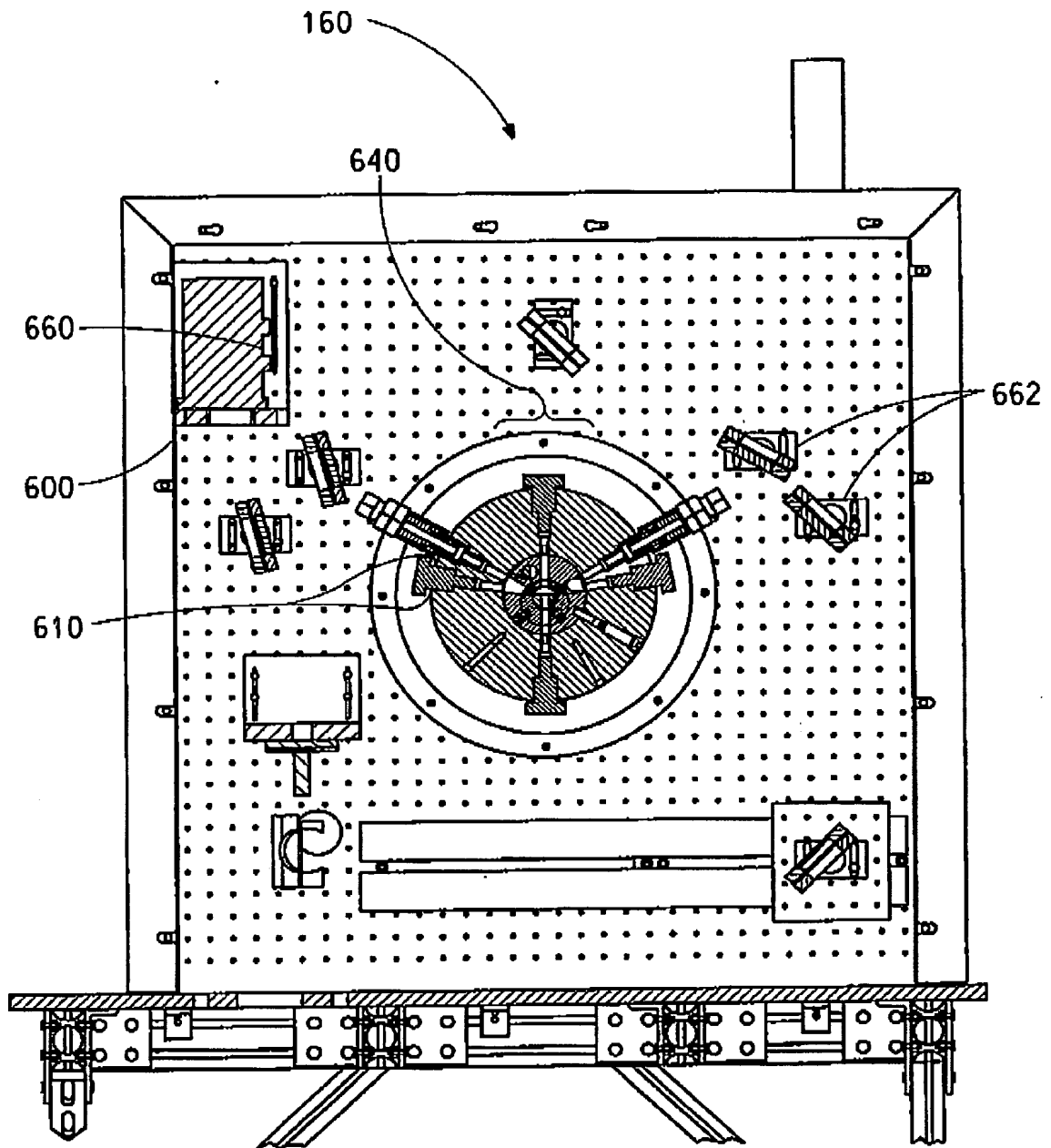


FIG. 5

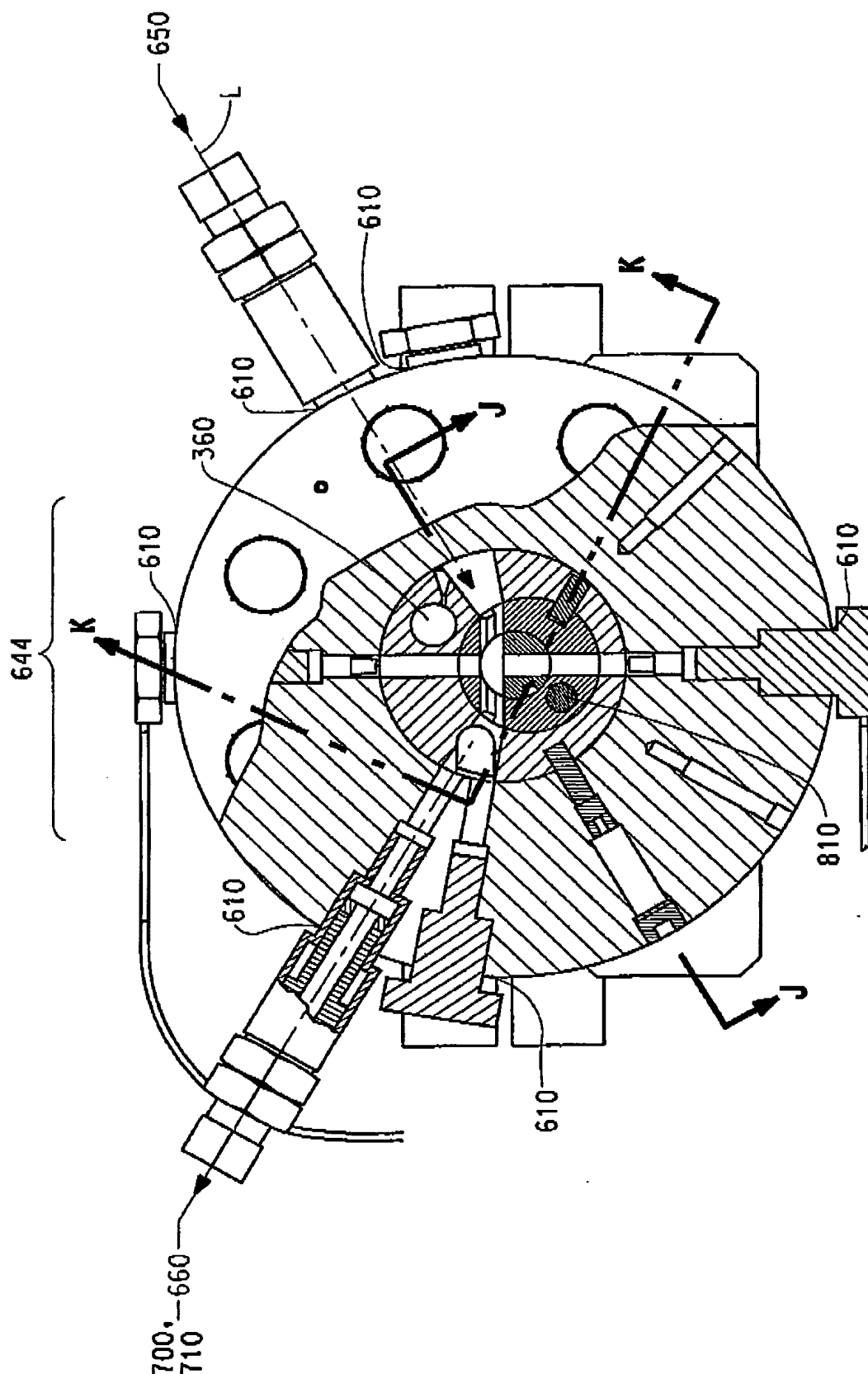
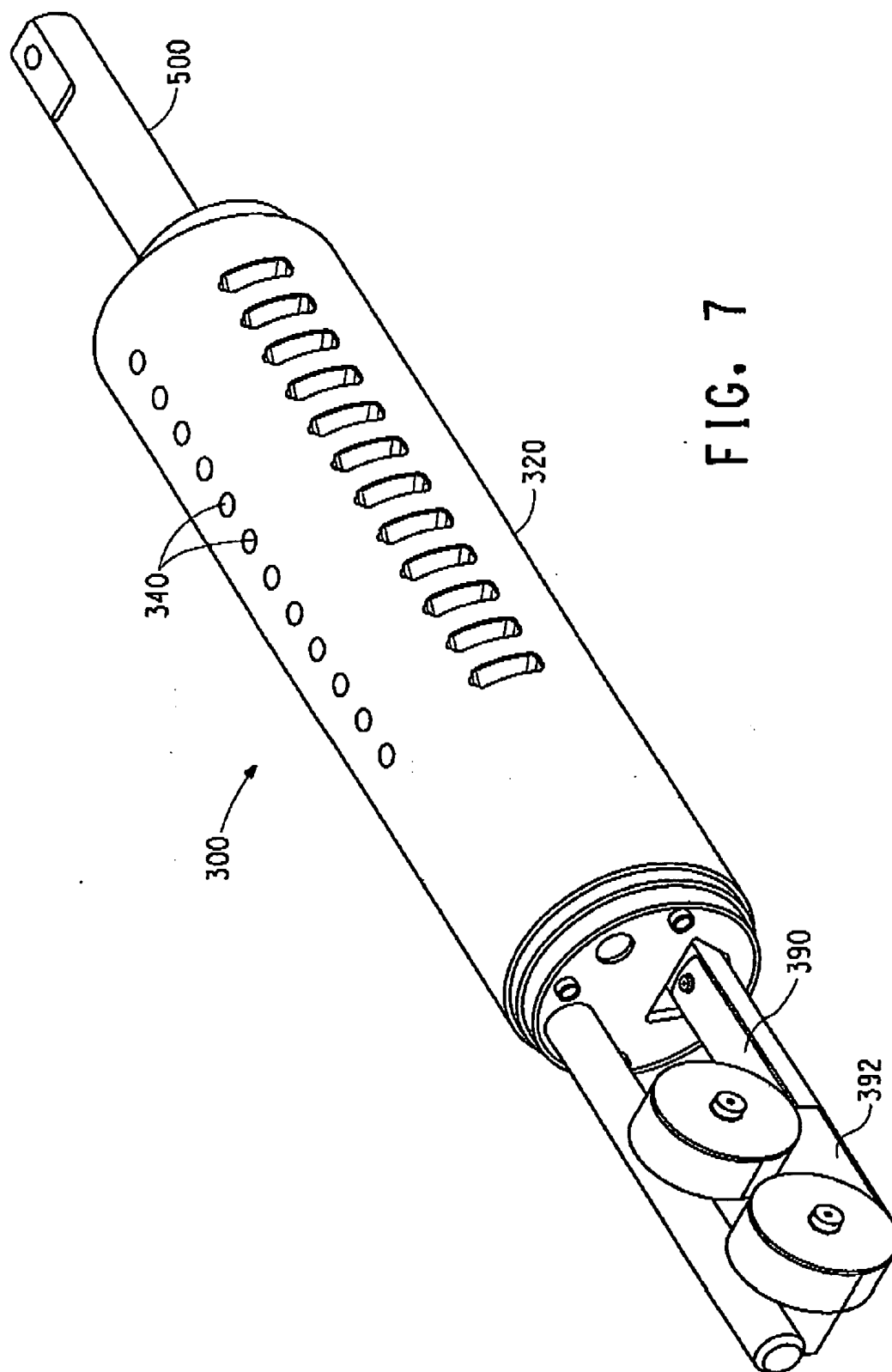
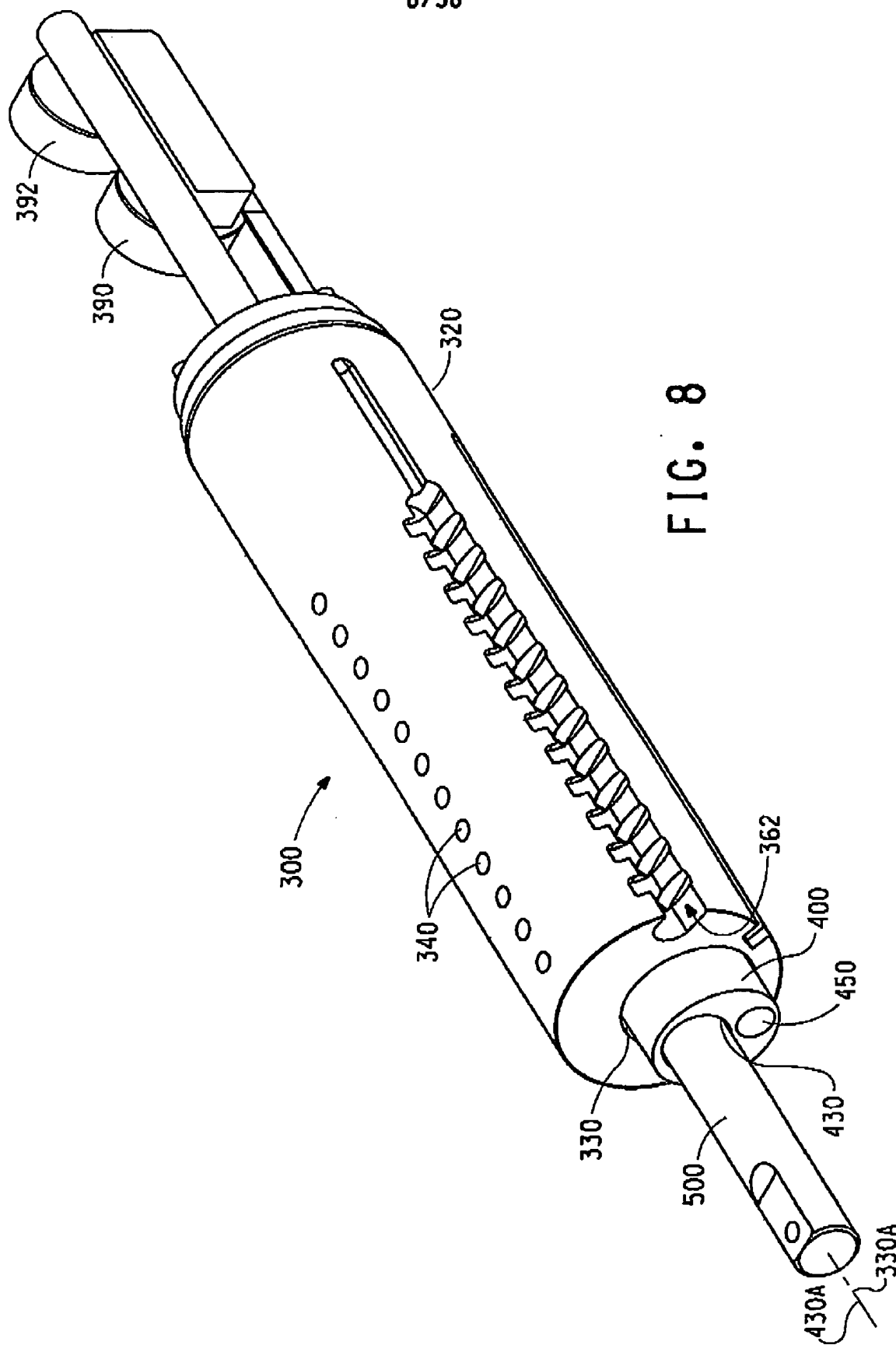


FIG. 6





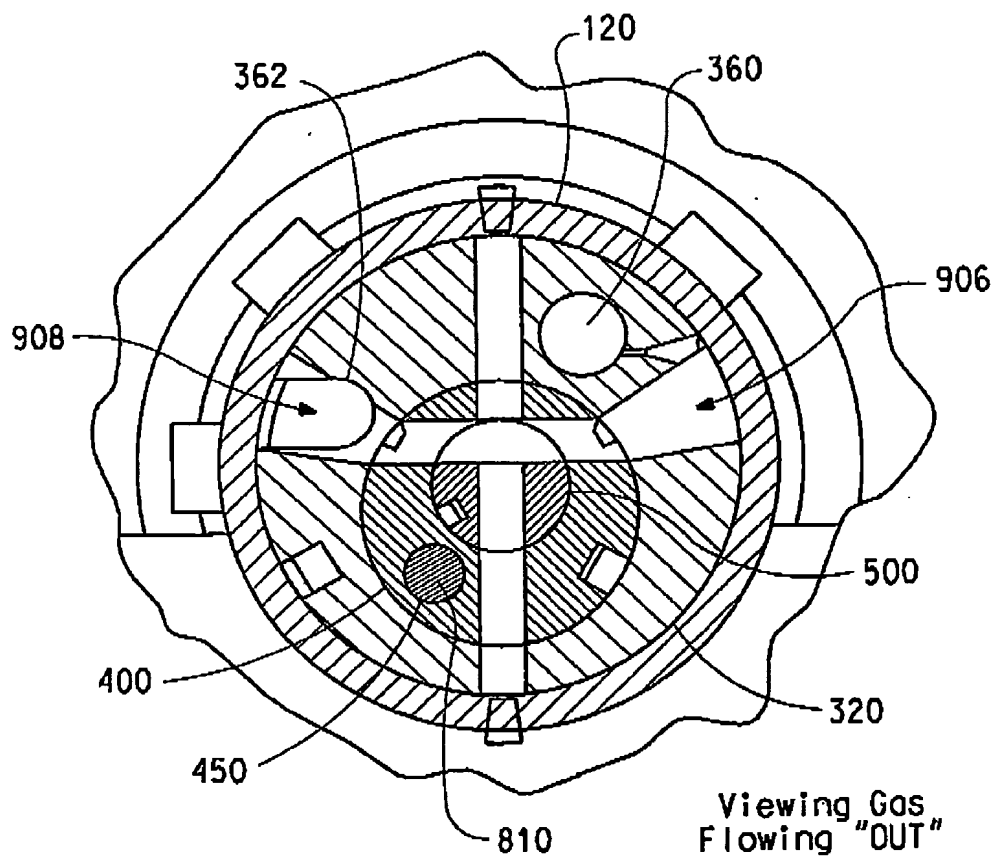


FIG. 9

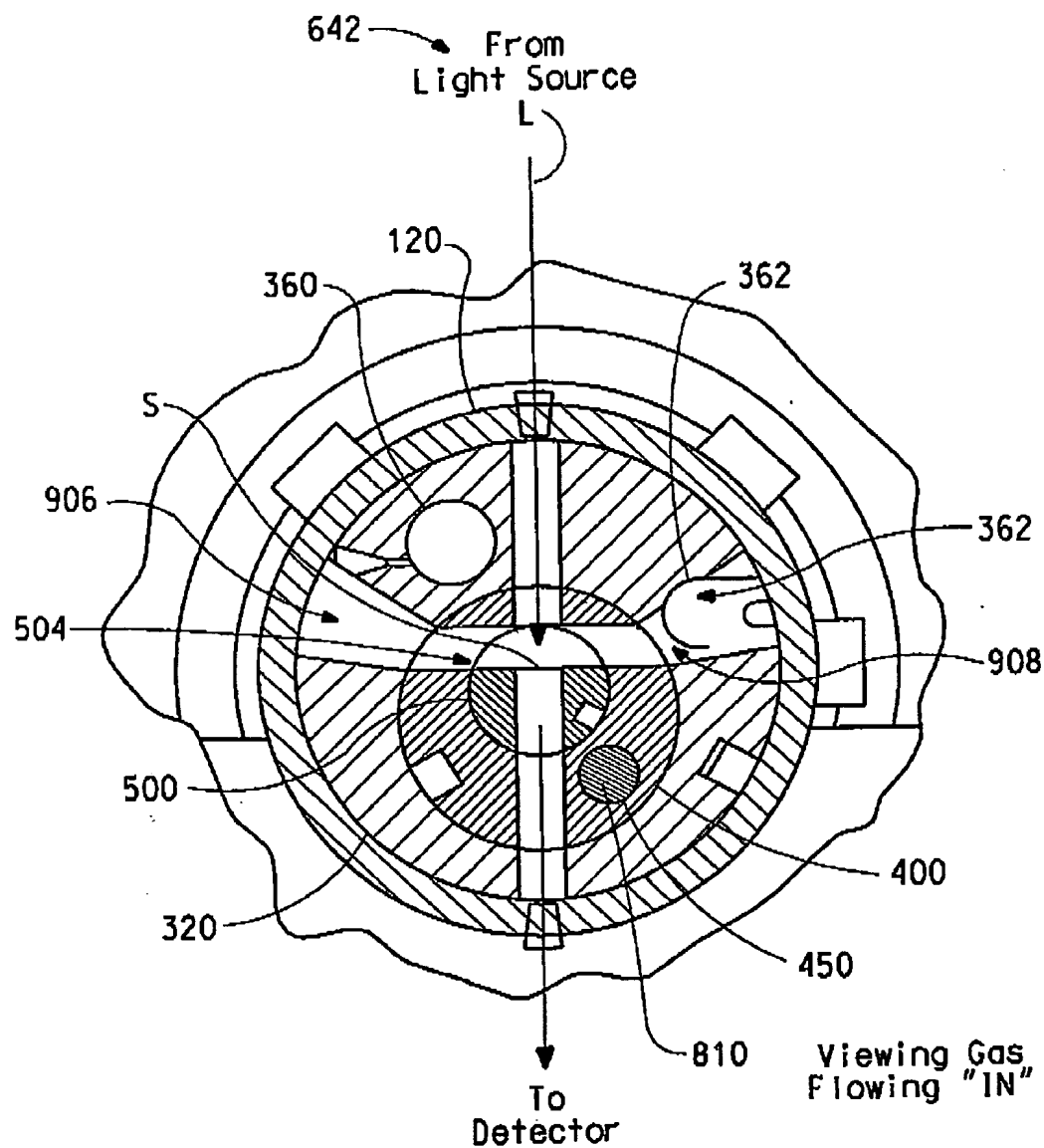


FIG. 10

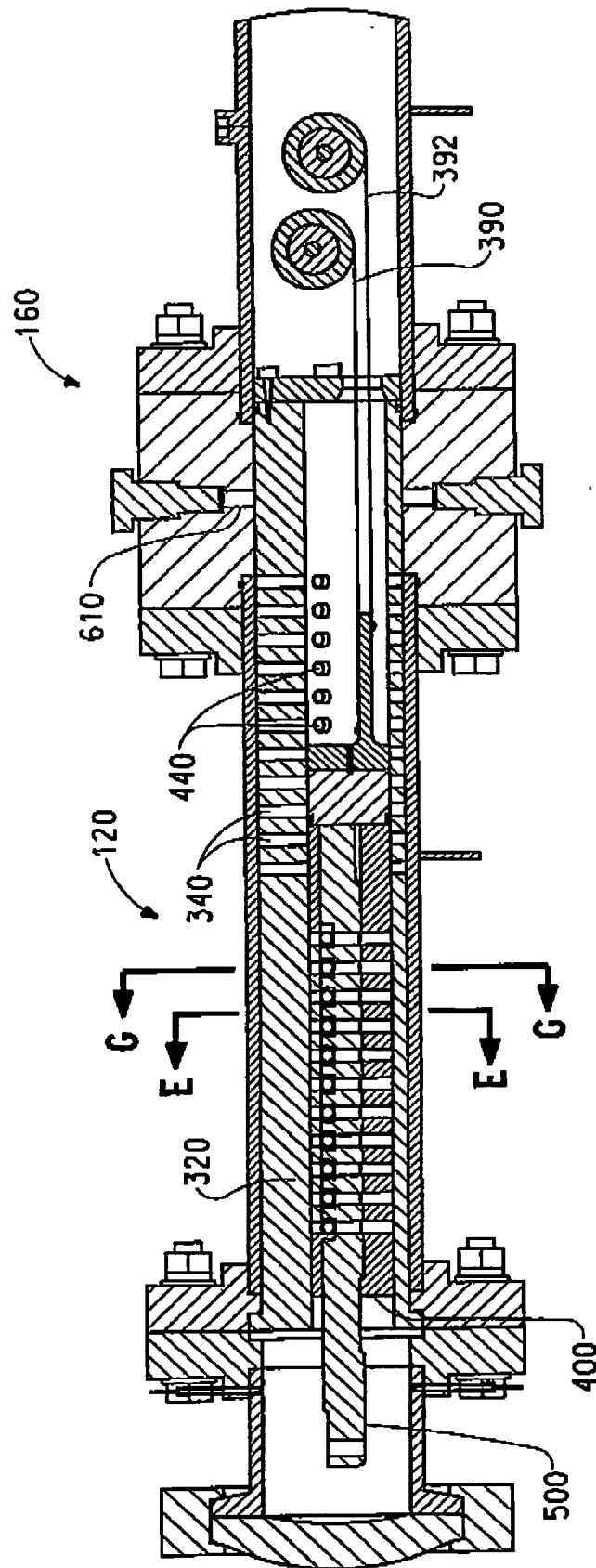


FIG. 11

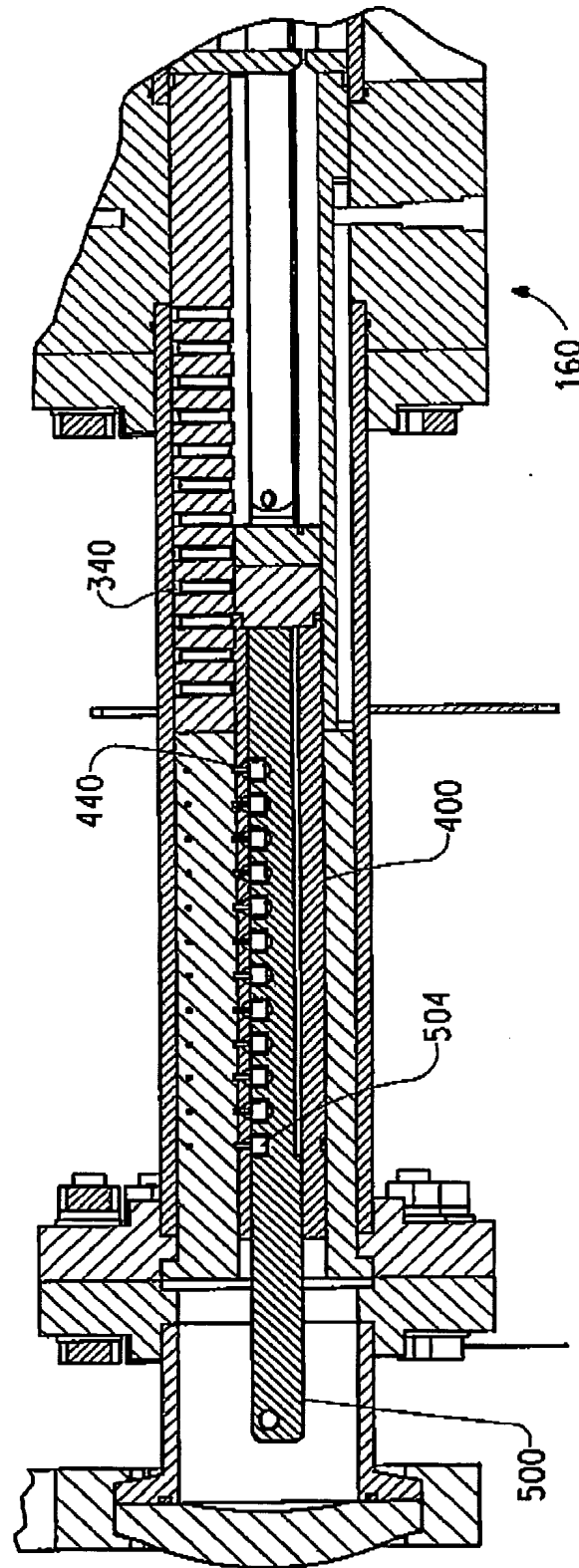


FIG. 12

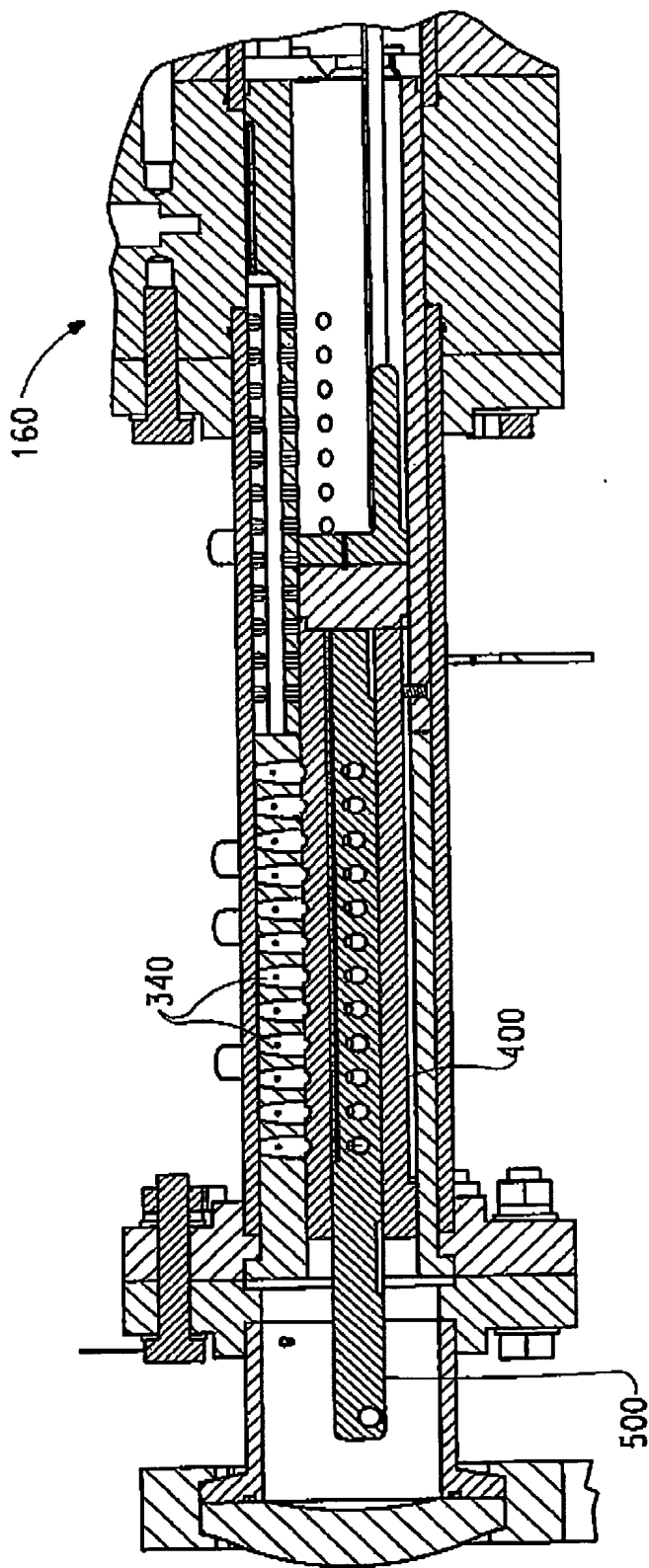


FIG. 13

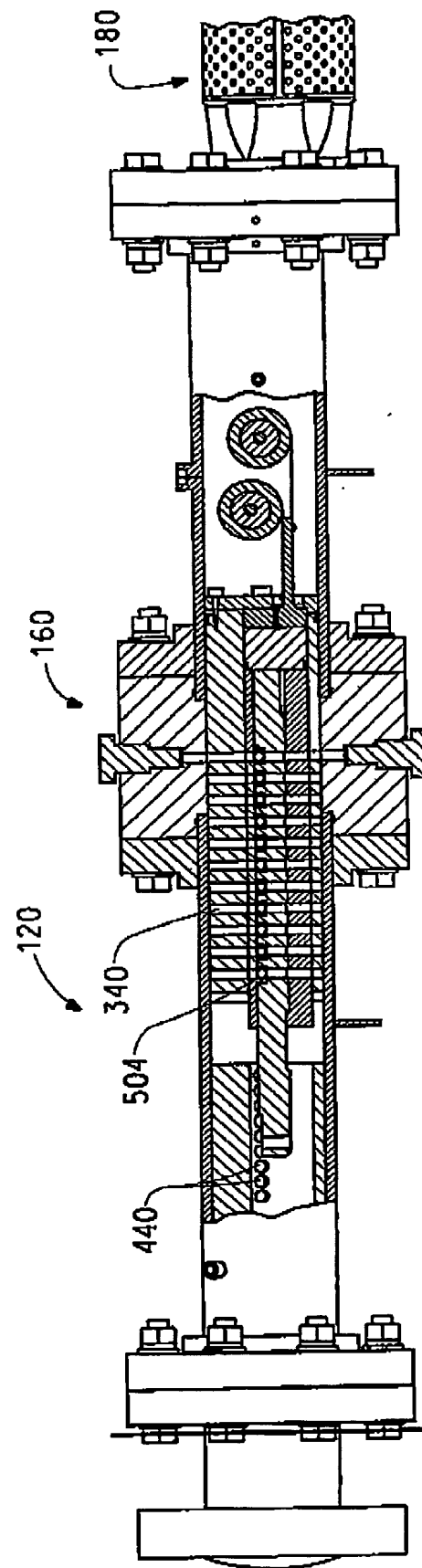


FIG. 14

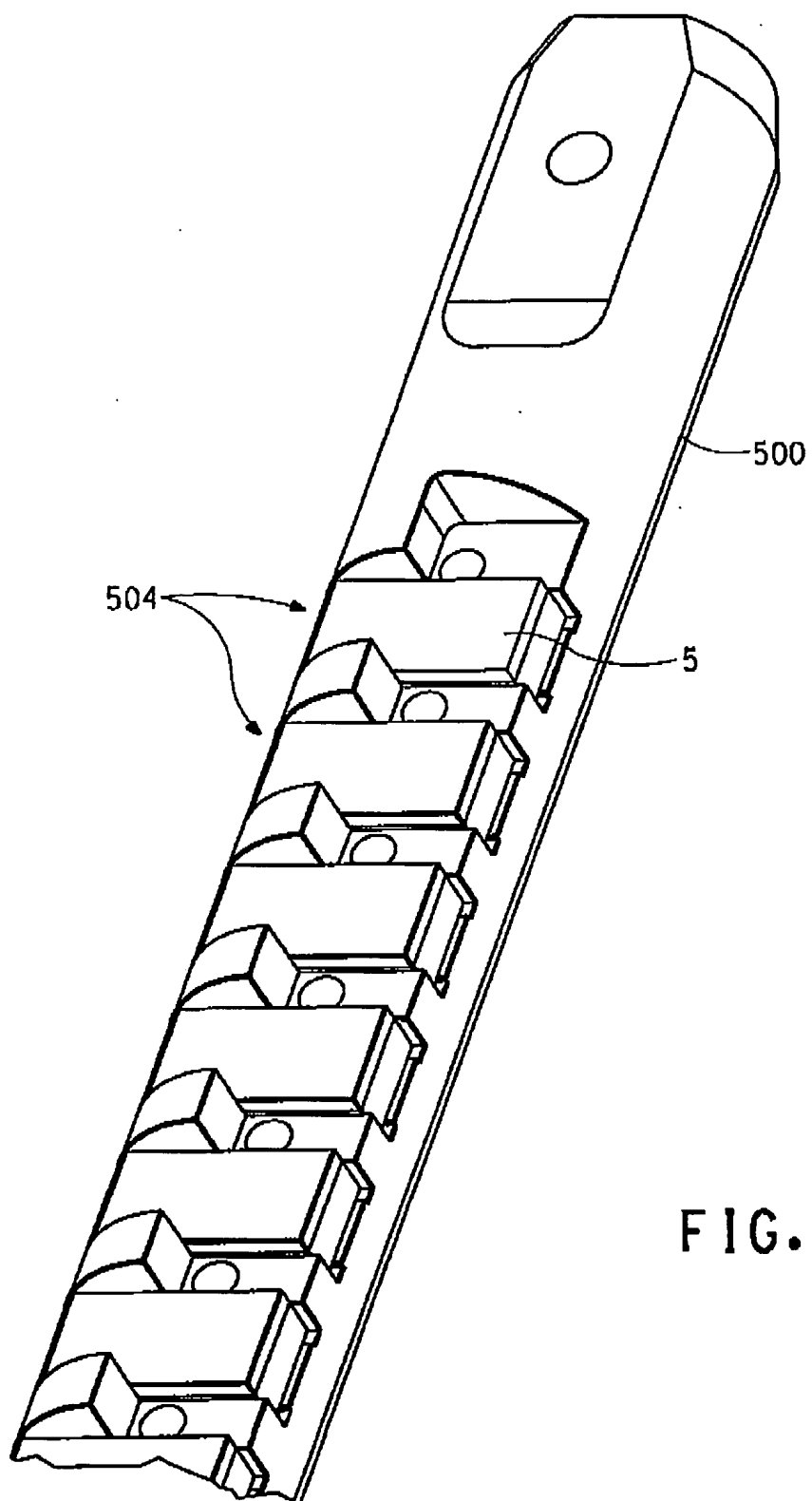


FIG. 15

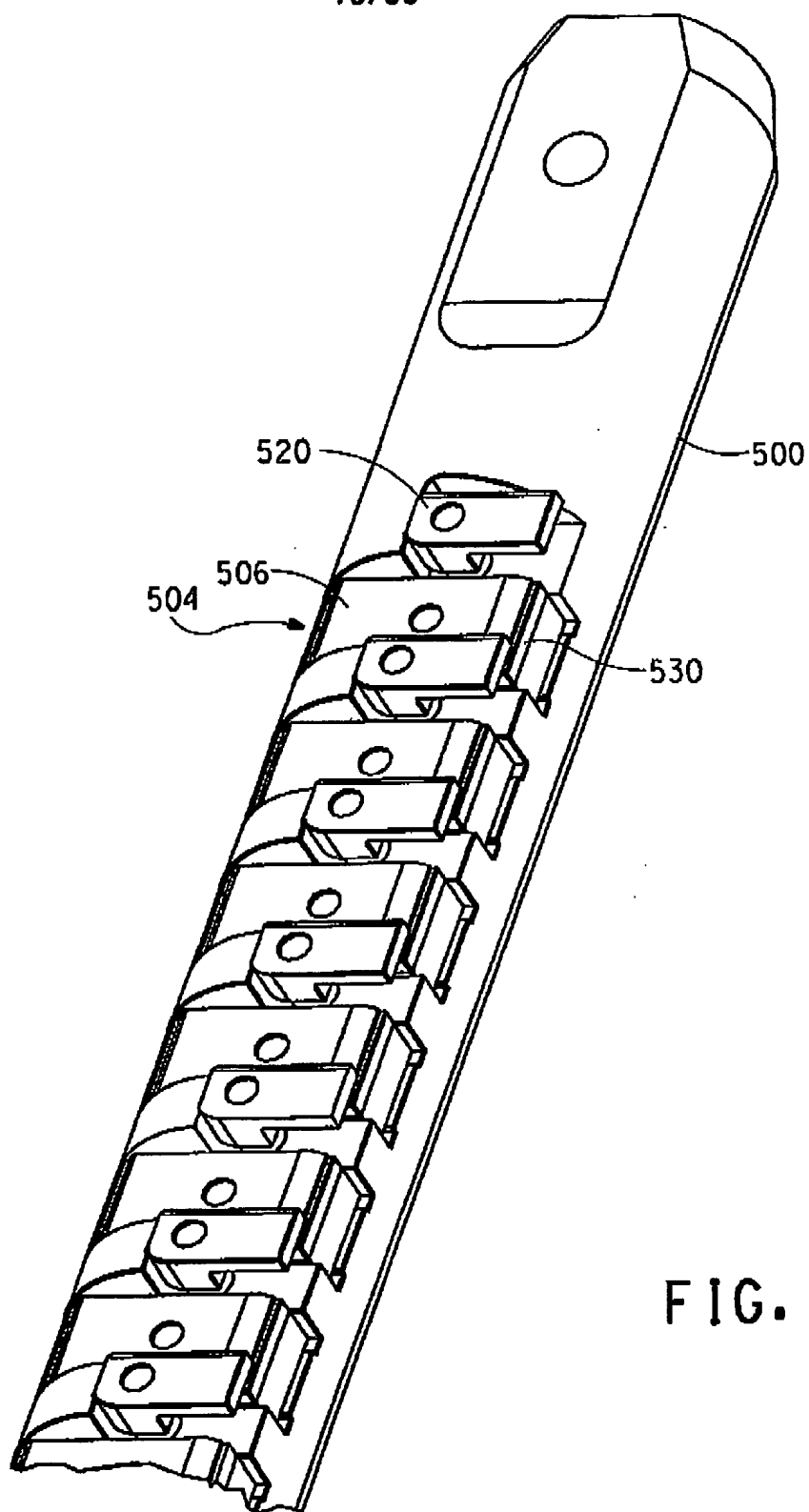
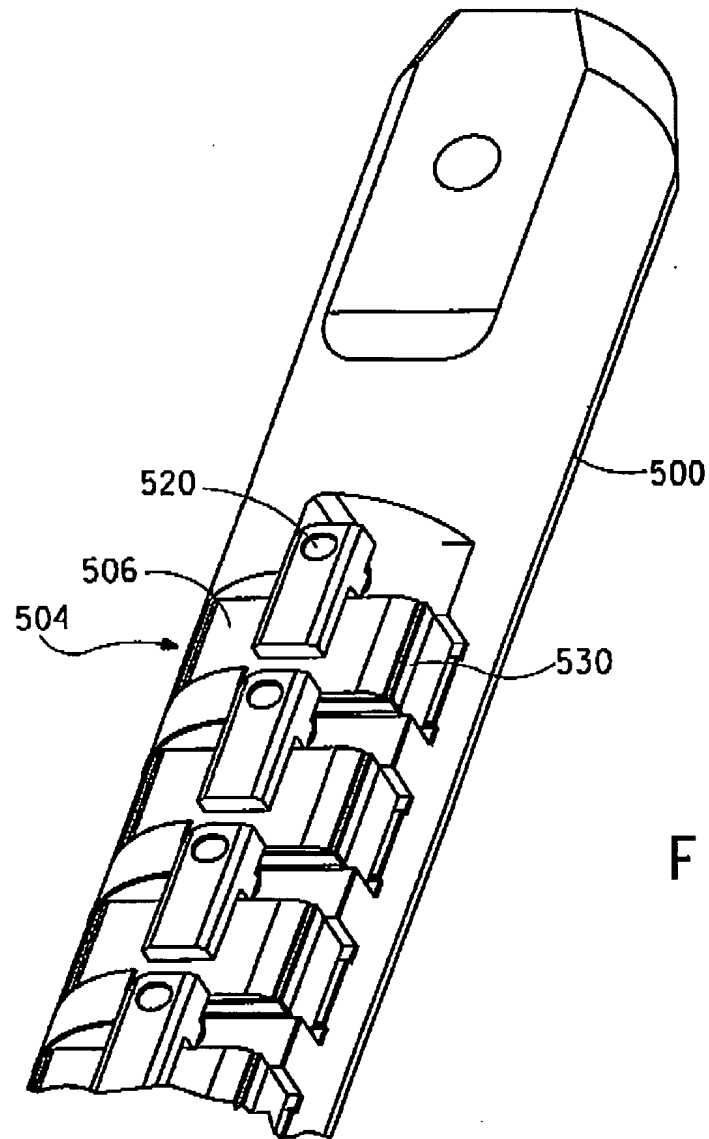


FIG. 16A



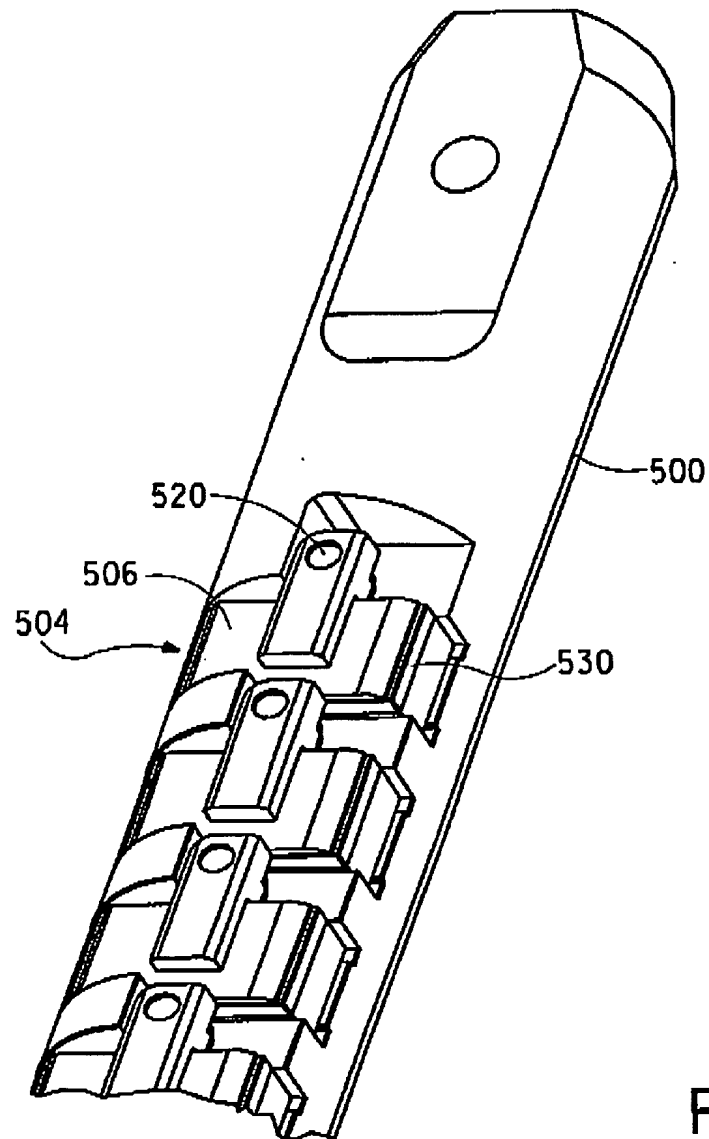


FIG. 16C

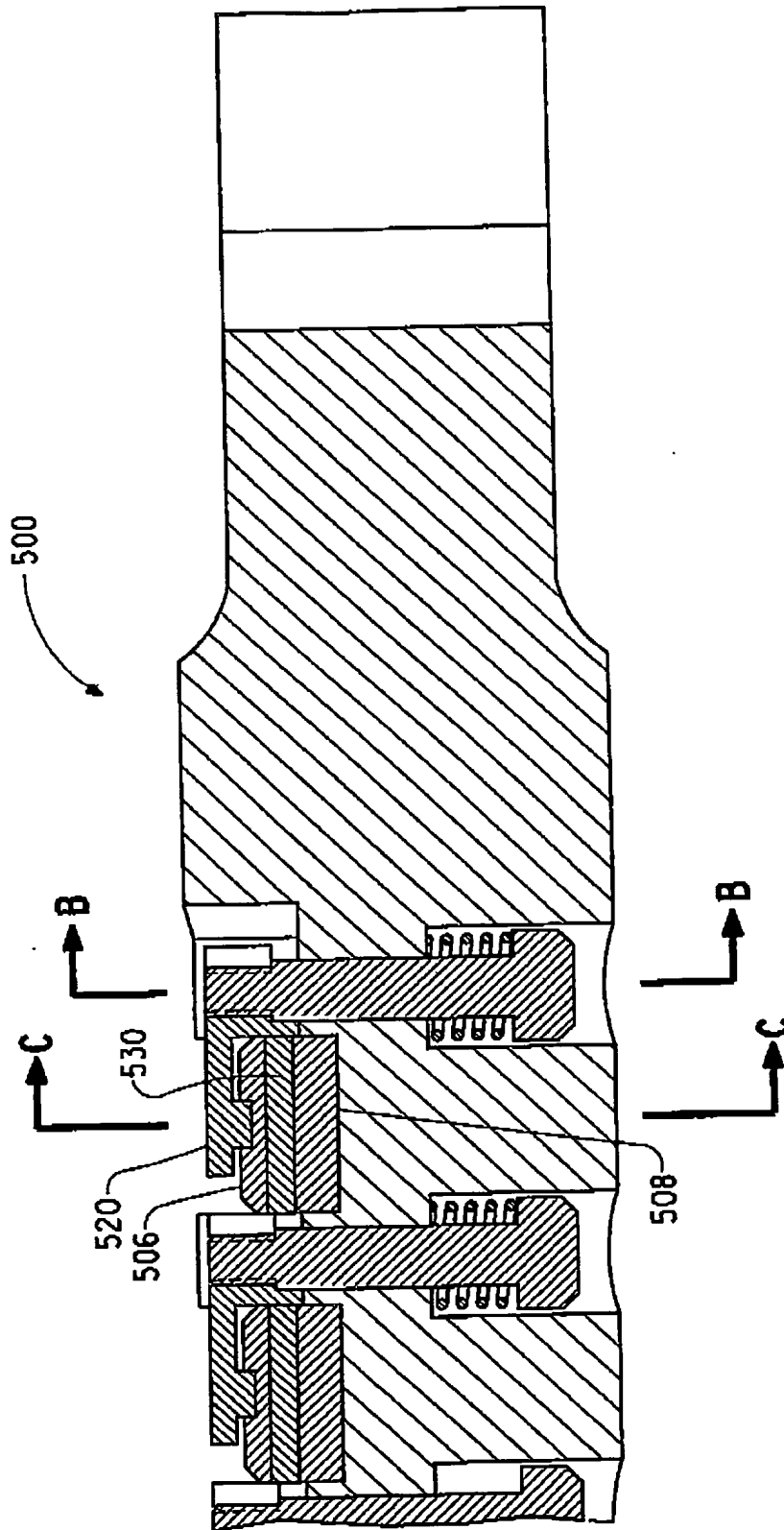


FIG. 17

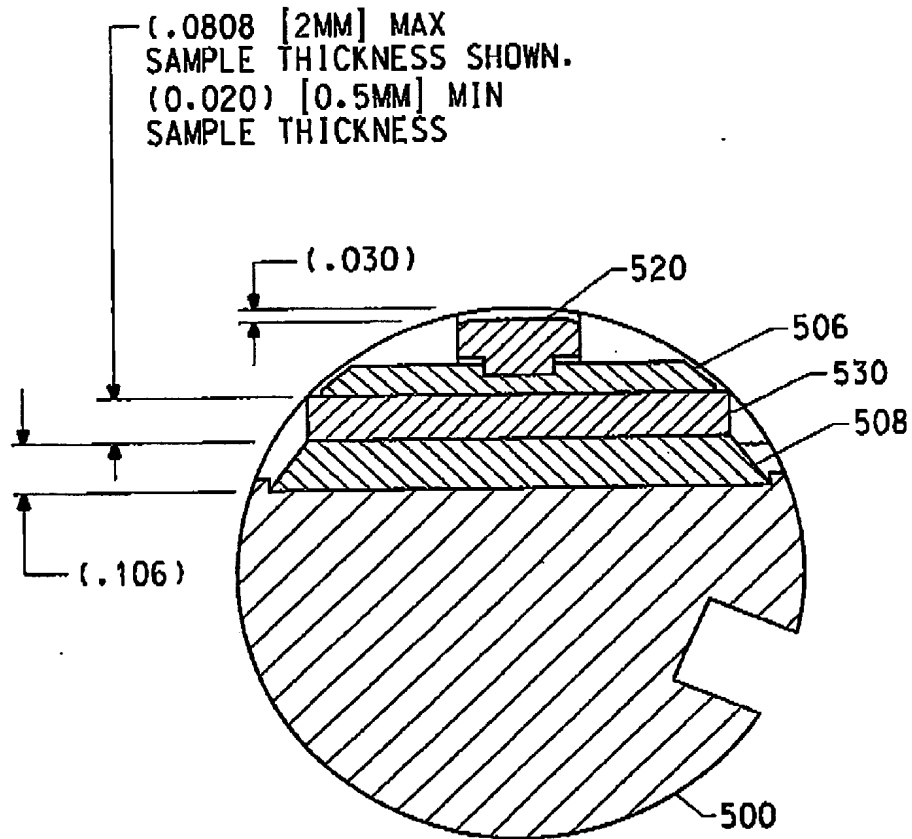


FIG. 18

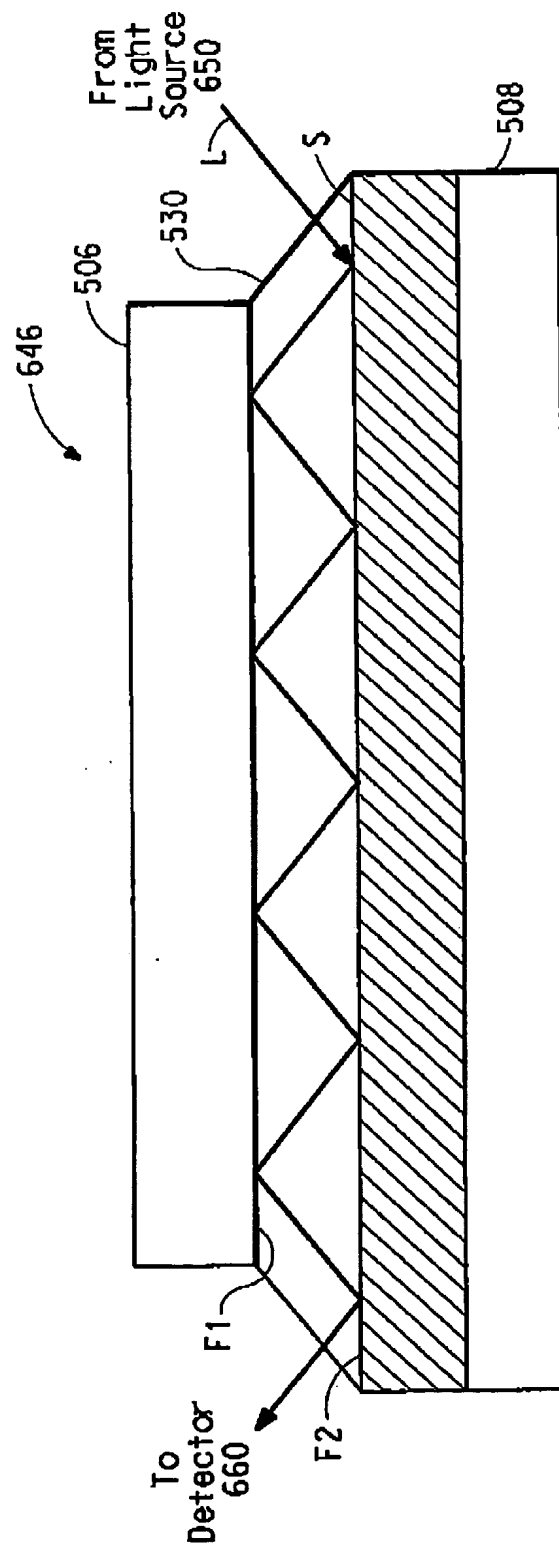


FIG. 18A

## FIG. 19A

### BUTTON SETUP

Button Set Points

Form Set Points

Function Activate Omegas

Initiates software communication link between this application and the temperature controllers for the reactor and process

Function Save Set Points

The user enters the temperature set point, maximum safety limit temperature and check box to activate each temperature zone in the reactor or process. This function then stores these settings as the new defaults as well as in records describing the experiment.

Function Send Set Points

Sends the temperature set points, safety limits and enable flag data to the temperature controller.

Function Dismiss

Removes this form window from the computer screen.

Button DataPath

Form DataPath

Function Make Directory

Creates a new directory to store data files and records associated with an experiment.

Continued on Fig. 19B

## FIG. 19B

Continued from Fig. 19A

### Function Apply

Sets the storage directory for data files as the path selected in the displayed directory box.

### Function Dismiss

Removes this form window from the computer screen.

### Button Motor

### Form Motor

### Function Go

Directs the motor to send the sample position to the optical measurement position.

### Function Go To Load Position

Directs the motor to send the sample canoe to the load position.

### Function Record Settings

Stores in memory which sample positions will be observed/skipped during an experimental run loop.

### Function Update Status

Updates the displayed status attributes of the motor, such as permission to move, current position, limit indicators, position error, motor overheating and motor power.

Continued on Fig. 19C

## FIG. 19C

Continued from Fig. 19B

### Function Stop Motor Now

Sends an immediate message to the positioning motor to stop moving.

### Function Dismiss

Removes this form window from the computer screen.

### Button Calibrate Motor

#### Form Calibrate motor

### Function Update Status

Updates the displayed status attributes of the motor, such as current location, home limit indicator, permission to move and position error.

### Function Go

Directs the motor to send the selected sample position to the optical measurement position.

### Function Set Sample Location @ Current

Stores in memory the current absolute motor position as the location at which the selected sample position is in the optical measurement position.

### Function Nudge the Motor

Directs the motor to move the sample canoe in the relative direction and distance indicated by the slider.

### Function Stop Motor Now

Sends an immediate message to the positioning motor to stop moving

Continued on Fig. 19D

## FIG. 19D

Continued from Fig. 19C

### Function Go There

Directs the motor to move the sample canoe to the absolute position entered in the text box.

### Function Find Diode

Directs the motor to move the sample canoe toward the reactor opening and stop when it reaches the home diode indicator.

### Function Find Load position

Same as Find Diode, but also travels to the load position, where the samples are positioned in the load/unloading gas manifold.

### Function Record All Parameters and Reset Motor

Stores all motor control parameters and positions in a permanent configuration file and sends these parameters to the motor memory.

### Function Read Control Parameters

Reads the current motor parameters in the motor memory. Displays these values in a new pop-up window.

### Function Dismiss

Removes this form window from the computer screen.

## FIG. 20A

**Button Ocean Optics**

**Form Ocean Optics**

**Function Correct Dark**

Activates internal circuitry in the UV/Vis spectrometer to correct for purely-electronic, dark signal error.

**Function View Test**

Collects all immediate UV/Vis spectrum and displays the spectrum in a pop-up window.

**Function Apply Settings**

Stores UV/Vis spectrometer settings entered in the form to the spectrometer hardware, computer memory and configuration files.

**Function Dismiss**

Removes this form window from the computer screen.

**Button Nicolet**

**Form Nicolet**

**Function Bench Set Up**

Activates FTIR spectrometer software to configure the FTIR processor, optical assembly and associated hardware.

**Function Invoke OMNIC**

Activates vendor FTIR software for data visualization and processing.

Continued on Fig. 20B

## FIG. 20B

Continued from Fig. 20A

### Function Apply Settings

Stores all FTIR spectrometer settings entered in the form to the spectrometer hardware, computer memory and configuration files.

### Function Dismiss

Removes this form window from the computer screen.

## FIG. 21A

Button Parameters

Form Parameters

Button Set Path

Form DataPath

Function Write Experiment File

Records all parameters and settings in a configuration file which would be required to describe and reproduce exactly the current experiment.

Button Head Settings Experiment File

Opens the Read Setting Experiment File form.

Form Read Settings Experiment File

Function Read

Restores a complete set of parameters and settings from the previously written experiment file displayed in the file directory box.

Function Read + Set Path

Same as Function Read, but also sets the directory to store new data as the same directory as the experiment file to be selected and read

Function Dismiss

Removes this form window from the computer screen.

Continued on Fig. 21B

## FIG. 21B

Continued from Fig. 21A

### Button Set Motor Positions

#### Form Motor

#### Function Refresh

Updates the listing of all experimental setting and parameter values listed in the text area in the upper right section of this form.

#### Function Dismiss

Removes this form window from the computer screen.

## FIG. 22

### Button Configuration

#### Form Configuration

#### Function Record These Ports

Permits the user to assign computer serial port numbers to the interfaced instrumentation, such as the motor, UV/Vis spectrometer, temperature controllers and analog/digital signal converter

#### Function Record These Names

Permits the user to assign zone names to pressure and temperature sensing signals.

#### Function Check Installation

Runs a test to ensure the software and its requisite resources are installed, configured and working properly.

#### Function Dismiss

Removes this form window from the computer screen.

## FIG. 23A

### Button Process

#### Button Open/Close Valves

#### Form Open/Close Valves

#### Function Send

Transmits signals to the solenoids to either open or close the Load In and Load Out valves, depending on the radio button selections on the form.

#### Function Dismiss

Removes this form window from the computer screen.

### Button SetPoints

#### Form SetPoints

#### Button Show Process

#### Form Show Process

#### Function Update

Displays the current temperature and pressure zone names and attributes, such as control set point, current value, maximum limit, enable status and heating power output.

#### Function Dismiss

Removes this form window from the computer screen.

Continued on Fig. 23B

## FIG. 23B

Continued from Fig. 23A

### Function Auto-Tune Omegas(!)

Initiates the temperature controller firmware which begins heating the process zones while computing optimal PID controller parameters

### Function Show Process Logs

Displays a pop-up window which displays the recent history of process temperatures, process pressures, system messages and experimental events.

## FIG. 24A

### Button Experiment

#### Button Parameters

##### Form Parameters

#### Button Apply

##### Function Apply

Updates and records all parameters and settings in memory which would be required to describe and reproduce exactly the current experiment.

### Button Run !!

#### Function Run

Activates the automated run sequence for an experiment. The run sequence is displayed in the Parameters form.

### Button Pause

#### Function Pause

Pauses the automated run sequence or Resumes the current run sequence.

### Button Data

#### Button View IR Spectrum

##### Function View IR Spectrum

Activates vendor software to display and analyze a recorded FTIR spectrum.

Continued on Fig. 24B

## FIG. 24B

Continued from Fig. 24A

### Button Analyze IR Series

#### Form Analyze IR Series

##### Function Select

Use the data in the file currently selected in the file list box as a background reference to compute new peak heights and areas.

##### Function View

Display the data in the file currently selected in the file list box as a spectrum with the previously selected background reference. The user may select regions to define the appropriate baseline and peak integration limits.

##### Function Apply

Record and use the previously selected baseline and peak integration limit.

##### Function Process

For the data in each file over the range of files selected in the form, integrate the absorbance peak using the background, baseline and limit specifications displayed in the form. Write the collection time and peak area data in a result file.

Continued on Fig. 24C

## FIG. 24C

Continued from Fig. 24B

### Function View Data

Invoke a Notepad editor to view the aforementioned result file.

### Function Dismiss

Removes this form window from the computer screen.

### Button Export IR Series

#### Form Export IR Series

### Function Make Dir

Create a new directory in which will be generated.

### Function Run

Convert the data in the selected file sequence from their current data format into the format selected in the list box. Store each data file set in a new file with the same file name and new format suffix.

### Function Dismiss

Removes this form window from the computer screen.

## FIG. 25A

**Button View UV/Vis Spectrum**  
**Function Invoke UV/Vis**

Begin the execution of a program to view UV/Vis spectra recorded during a previous experiment.

**Button Analyze UV/Vis Series**  
**Function Invoke UV/Vis**

Begin the execution of a program to analyze UV/Vis spectra and absorptions recorded during a previous experiment.

**Button Export UV/Vis Series**  
**Function Invoke UV/Vis**

Begin the execution of a program to convert data in one format to another.

**Button Set Motor's Home Position**  
**Form Set Motor's Home Position**  
**Button Sample Boat is Intalled**  
**Function Sample Boat is Installed**

Motor is safe to operate. The function begins a sequence to find the sample canoe standard load position. If the sequence is successful, permission is granted to move the motor.

**Button Cancel**  
**Function Cancel**

The user selects this button when he cannot confirm that the sample boat is properly loaded. The software does not set the home position and does not grant permission to move the motor.

Continued on Fig. 25B

## FIG. 25B

Continued from Fig. 25A

**Button Emergency Motor Stop**

**Function Emergency Motor Stop**

The motor is sent an immediate message to stop motion, the experiment is terminated and the program is terminated.

**Button Exit and Kill**

**Form Exit and Kill**

**Function Exit**

The user confirms that he wishes to terminate the program.

**Function Cancel**

Removes this form window from the computer screen.

## FIG. 26

### KEY:

The Software follows the familiar windows, event-driven mode of operation. The software does nothing until the user presses a button. The button pressing event may alter the viewable buttons or activate Forms and Functions. Forms and Functions are encoded as software subroutines. The various buttons and functions are identified by the label observed by the user on the forms.

### Form

A form presents a window on the user's computer screen. This form may present information, controls, input objects (such as text boxes, radio buttons, menus, lists, sliders), pictures, and command buttons.

### Button

A button (or command button) is pressed to execute a software command. The button typically begins the execution of a function, but may also expose new forms or replace the current set of viewable buttons.

### Function

A function initiates the execution of a software module which is typically a Visual Basic subroutine or function.